

Magnetic effect from non-magnetic impurity in superconducting CuO₂ plane

V.M. Loktev*

Bogolyubov Institute for Theoretical Physics, 14b Metrologichna str., 03143 Kiev-143, Ukraine

Yu.G. Pogorelov†

*CFP/Departamento de Fisica, Universidade do Porto,
Rua do Campo Alegre 687, 4169-007 Porto, Portugal*

We propose a new model for impurity center formed by a cation substitute for Cu, like Zn, in CuO₂ planes. Its main effect on superconducting electrons is due to the non-zero exchange field on O sites, neighbors to the (non-magnetic) impurity. We discuss a strong suppression of *d*-wave order parameter, a zero-energy resonance in local density of states, and spin polarization of charge carriers, which can be related to the experimentally observed effects in Zn-doped copper oxides. These results are obtained *without* using the unitary scattering limit.

It is recognized that there are two types of impurities in high-T_c superconductors (HTSC): i) intrinsic or “own”, and ii) extrinsic or “foreign”. The first type are the heterovalent impurities or oxygen vacancies, that is the dopants. They supply charge carriers into insulating antiferromagnetic (AFM) cuprate planes enabling their metallization [1], but also they act as scattering centers for carriers. Previously, we showed [2, 3, 4] that formation of superconducting (SC) condensate, either of *s*- and *d*- symmetry, is possible at low enough concentration *c* of such impurities but is prevented by growing fluctuations of SC order parameter at higher *c*.

The second type are the homovalent impurities, which only produce scattering of existing charge carriers and so can depress the SC properties of HTSC systems. They are well studied in common SC metals, where it was stated by Anderson [5] that non-magnetic impurities have practically no effect on SC characteristics. At the same time, even low concentration of paramagnetic ions can completely destroy SC order, as initially shown in the Born approximation by Abrikosov and Gor’kov [6] and then confirmed by many authors under more general scope [7, 8, 9].

But in the case of SC copper oxides, an apparent violation of this so well theoretically based phenomenological principle was detected. Thus, introducing of non-magnetic Zn²⁺ ions instead of Cu²⁺ into the cuprate planes has a suppression effect on HTSC not weaker but rather stronger than that by magnetic Ni²⁺ ions [10, 11]. This triggered an idea of viewing the non-magnetic impurity ions in HTSC as extremely strong scatterers [12] so that their perturbation potential V_{imp} is the biggest energy parameter, treated in the unitary limit: $V_{imp}/W \gg 1$ (W the bandwidth). This concept was extensively elaborated [13, 14, 15], the principal conclusions being the finite density of quasiparticle states (DOS) at the Fermi level ε_F : $\rho(\varepsilon \rightarrow \varepsilon_F) \rightarrow \rho_u \neq 0$, and the universal value of

quasiparticle conductivity $\sigma(\omega \rightarrow 0) \rightarrow \sigma_u \neq 0$. However, apart from the still existing controversies about those predictions [16], it should be noted that, unlike the dopants, the foreign impurity centers are formed in the CuO₂ plane by a *homovalent* substitution (as Zn²⁺ or Ni²⁺ for Cu²⁺), and it is problematic how they could produce such a strong perturbation potential. Also we notice that the heterovalent non-magnetic scatterers by dopants can not produce such effects [3].

This Letter is aimed on an alternative approach to the problem of foreign impurities. It will be shown that irrespectively of the type (magnetic or non-magnetic) of the cation substitute in CuO₂ plane, the resulting center acts on charge carriers as *magnetic*. In accordance with the generally accepted notion, such center should in fact strongly suppress SC order either of *s*- or *d*-type, as was first qualitatively stated yet by Mahajan *et al* [17]. We note that similar views on the effect of Zn impurities in HTSC cuprates were expressed in some recent publications [18, 19, 20], though still focused on unitary scattering. Below we consider the problem of isolated non-magnetic impurity ion in a CuO₂ plane and its local effects on the *d*-wave SC order parameter, local density of states (LDOS), and the itinerant spin polarization. Our treatment does not need using the unitary limit, nevertheless the effects can be quite strong.

Fig. 1 shows a cation impurity substitute for Cu in a CuO₂ plane, like real Zn, Fe, or Ni impurities in high-T_c compounds. Associating the charge carriers mostly to O⁻ holes, we conclude that the main perturbation by such impurity (both magnetic and non-magnetic) is due to the fact that its neighbor O sites occur in a non-zero exchange field by Cu²⁺ ions [21, 22], which is equivalent to the effect of magnetic impurity in a common superconductor. On the other hand, there are no reasons to consider any sizeable spin-independent perturbation from such isovalent impurity. The respective model Hamiltonian is $H = H_{sc} + H_c + H_{int}$. The unperturbed SC term $H_{sc} = \sum_{\mathbf{k}} \psi_{\mathbf{k}}^\dagger (\xi_{\mathbf{k}} \hat{\tau}_3 + \Delta_{\mathbf{k}} \hat{\tau}_1) \psi_{\mathbf{k}}$ couples the Nambu spinors $\psi_{\mathbf{k}}^\dagger = (a_{\mathbf{k},\uparrow}^\dagger, a_{-\mathbf{k},\downarrow})$ with Pauli matrices $\hat{\tau}_i$. The normal dispersion $\xi_{\mathbf{k}} = W(2 - \cos ak_x - \cos ak_y)/4 - \varepsilon_F$ leads to the density of states (DOS) $\rho_0 = 4/(\pi W)$. The *d*-wave

*Electronic address: vloktev@gluk.org

†Electronic address: ypogorel@fc.up.pt

gap function $\Delta_{\mathbf{k}} = \Delta\theta(\varepsilon_D^2 - \xi_{\mathbf{k}}^2)\gamma_{\mathbf{k}}/\gamma_m$ includes the BCS-shell factor $\theta(\varepsilon_D^2 - \xi_{\mathbf{k}}^2)$ with the “Debye energy” ε_D , the symmetry factor $\gamma_{\mathbf{k}} = \cos ak_x - \cos ak_y$ with maximum absolute value $\gamma_m = \pi\varepsilon_F\rho_0$, and the gap parameter

$$\Delta = VN^{-1} \sum_{\mathbf{k}} \gamma_{\mathbf{k}} \langle a_{-\mathbf{k},\downarrow} a_{\mathbf{k},\uparrow} \rangle \quad (1)$$

where V is the attraction between two carriers with opposite spins on neighbor O sites. The term $H_c = -hS_z$ models the (AFM) correlation between the impurity center and its environment, where $h \sim J_{dd}$, the Cu-Cu exchange constant, and \mathbf{S} is the spin of a fictitious “magnetic impurity”. It can be seen as a cluster of four $1/2$ spins of Cu nearest neighbors to real non-magnetic impurity (Fig. 1). In reality, its quantization axis z is only defined over time periods no longer than $\tau_s \sim \hbar\xi_s/(aJ_{dd}) \sim 10^{-13}$ s for spin correlation length $\xi_s \sim a/\sqrt{x}$ [23] and doping levels $x \sim 0.1$ (this also agrees with the NMR data [18]). However this τ_s is much longer than typical electronic times $\sim \hbar/\varepsilon_F \sim 10^{-15}$ s for HTSC compounds. For $h > 0$ we have $\langle S_z \rangle \equiv s$ and $0 < s < S$, which accounts for the short-range AFM order, whereas $s \rightarrow 0$ in the paramagnetic limit $\beta h \ll 1$.

We separate the spin-dependent interaction between charge carriers and impurity into three parts:

$$H_{int} = H_{int}^{MF} + H_{int}^{\parallel} + H_{int}^{\perp}, \quad (2)$$

where

$$H_{int}^{MF} = JsN^{-1} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma=\pm} \alpha_{j,\mathbf{k}} \alpha_{j,\mathbf{k}'} \sigma a_{\mathbf{k}',\sigma}^{\dagger} a_{-\mathbf{k},\sigma}$$

is the “mean-field” (MF) polarization of carrier spins by the impurity center, and

$$H_{int}^{\parallel} = JN^{-1} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma=\pm} \alpha_{j,\mathbf{k}} \alpha_{j,\mathbf{k}'} \sigma (S_z - s) a_{\mathbf{k}',\sigma}^{\dagger} a_{\mathbf{k},\sigma},$$

$$H_{int}^{MF} = JN^{-1} \sum_{\mathbf{k},\mathbf{k}'} \sum_{\sigma=\pm} \alpha_{j,\mathbf{k}} \alpha_{j,\mathbf{k}'} S_{\sigma} a_{\mathbf{k}',-\sigma}^{\dagger} a_{\mathbf{k},\sigma},$$

are their interactions with longitudinal and transversal fluctuations of \mathbf{S} . In the paramagnetic limit: $s \rightarrow 0$, Eq. 2 is reduced to the common Kondo interaction [24, 25]. For definiteness, the Cu-O p - d exchange parameter J is considered positive. The functions

$$\begin{aligned} \alpha_{1,\mathbf{k}} &= 2 \cos \frac{ak_x}{2} \cos \frac{ak_y}{2}, & \alpha_{2,\mathbf{k}} &= 2 \cos \frac{ak_x}{2} \sin \frac{ak_y}{2}, \\ \alpha_{3,\mathbf{k}} &= 2 \sin \frac{ak_x}{2} \cos \frac{ak_y}{2}, & \alpha_{4,\mathbf{k}} &= 2 \sin \frac{ak_x}{2} \sin \frac{ak_y}{2}, \end{aligned}$$

realize 1D irreducible representations of the C_{4v} point group (of the plaquette surrounding the impurity), so that $N^{-1} \sum_{\mathbf{k}} \alpha_{j,\mathbf{k}} \alpha_{j',\mathbf{k}} = \delta_{jj'}$. Distinctive features of the perturbation, Eq. 2, compared to the commonly used impurity models, are: i) its spatial extension expressed by

the factors $\alpha_{j,\mathbf{k}}$, ii) additional degrees of freedom by spin \mathbf{S} , and iii) coupling of \mathbf{S} to the local AFM correlations.

In principle, this impurity center can produce yet another perturbation, due to a possible role of AFM correlated Cu^{2+} spins in the SC coupling between charge carriers. Lacking one such spin would locally perturb the $\Delta_{\mathbf{k}}\hat{\tau}_1$ term in H_{sc} by some expansions in $\alpha_{j,\mathbf{k}}\alpha_{j,\mathbf{k}'}$. This can influence the SC order, alike the simpler case of point-like perturbation of s -wave SC coupling [26]. However, for simplicity, we leave this kind of perturbation for a separate study.

We calculate the averages, like Eq. 1, by simple spectral formula at $T = 0$:

$$\langle ab \rangle = \pi^{-1} \int_0^{\varepsilon_F} \Im \langle \langle b|a \rangle \rangle_{\varepsilon} d\varepsilon, \quad (3)$$

where $\Im f(\varepsilon) = \lim_{\delta \rightarrow 0} [f(\varepsilon - i\delta) - f(\varepsilon + i\delta)]/2$ and $\langle \langle b|a \rangle \rangle_{\varepsilon \pm i\delta}$ are the retarded and advanced two-time Green functions (GF's). The relevant GF matrix $\hat{G}_{\mathbf{k},\mathbf{k}'} = \langle \langle \psi_{\mathbf{k}} | \psi_{\mathbf{k}'}^{\dagger} \rangle \rangle$ in absence of impurity perturbation ($J = 0$) is momentum-diagonal: $\hat{G}_{\mathbf{k},\mathbf{k}'} = \delta_{\mathbf{k},\mathbf{k}'} \hat{G}_{\mathbf{k}}$, with $\hat{G}_{\mathbf{k}} = (\varepsilon - \xi_{\mathbf{k}}\hat{\tau}_3 - \Delta_{\mathbf{k}}\hat{\tau}_1)^{-1}$. The same expression holds for the momentum-diagonal GF $\hat{G}_{\mathbf{k},\mathbf{k}}$ in presence of single impurity, whose effect $\sim 1/N$ is negligible for this quantity. However it is only this small impurity effect that gives rise to a momentum-non-diagonal GF's $\hat{G}_{\mathbf{k},\mathbf{k}'}$. They are found from the equation of motion $\hat{G}_{\mathbf{k},\mathbf{k}'} = JN^{-1} \sum_{\mathbf{k}'',j} \alpha_{j,\mathbf{k}} \hat{G}_{\mathbf{k}} (s\hat{G}_{\mathbf{k}'',\mathbf{k}'} + \hat{G}_{\mathbf{k},\mathbf{k}'}^{(z)} + \hat{G}_{\mathbf{k},\mathbf{k}'}^{(-)}) \alpha_{j,\mathbf{k}''}$ including three scattered GF's: the MF one $\hat{G}_{\mathbf{k}'',\mathbf{k}'}$, the longitudinal $\hat{G}_{\mathbf{k}'',\mathbf{k}'}^{(z)} = \langle \langle \psi_{\mathbf{k}''} (S_z - s) | \psi_{\mathbf{k}'}^{\dagger} \rangle \rangle$ and the transversal $\hat{G}_{\mathbf{k}'',\mathbf{k}'}^{(-)} = \langle \langle \bar{\psi}_{\mathbf{k}''} S_- | \psi_{\mathbf{k}'}^{\dagger} \rangle \rangle$ with $\bar{\psi}_{\mathbf{k}}^{\dagger} = (a_{\mathbf{k},\downarrow}^{\dagger}, a_{-\mathbf{k},\uparrow})$. The two last terms are analogous to the well known Nagaoka's Γ -term [9, 25] and treating them with a similar decoupling procedure gives:

$$\begin{aligned} \hat{G}_{\mathbf{k},\mathbf{k}'}^{(z)} &= \frac{J\Sigma^2}{N} \sum_{\mathbf{k}'',j} \alpha_{j,\mathbf{k}} \hat{G}_{\mathbf{k}} \hat{G}_{\mathbf{k}'',\mathbf{k}'} \alpha_{j,\mathbf{k}''}, \\ \hat{G}_{\mathbf{k},\mathbf{k}'}^{(-)} &= \frac{J}{N} \sum_{\mathbf{k}'',j} \alpha_{j,\mathbf{k}} \hat{G}_{\mathbf{k}} (\varepsilon + h) \hat{X}_{\mathbf{k}'',\mathbf{k}'} \hat{G}_{\mathbf{k}'',\mathbf{k}'} \alpha_{j,\mathbf{k}''}, \end{aligned}$$

where $\Sigma^2 = \langle S_z^2 \rangle - s^2$, $\hat{X}_{\mathbf{k}} = S(S+1) - s(s+1) - \Sigma^2 + (1 + 2\xi_{\mathbf{k}}/E_{\mathbf{k}})\hat{\tau}_3$, $E_{\mathbf{k}} = \sqrt{\xi_{\mathbf{k}}^2 + \Delta_{\mathbf{k}}^2}$, and one energy argument is shifted: $\varepsilon \rightarrow \varepsilon + h$, due to the AFM stiffness. Finally, we obtain the decoupled equation of motion:

$$\hat{G}_{\mathbf{k},\mathbf{k}'} = N^{-1} \sum_{\mathbf{k}'',j} \alpha_{j,\mathbf{k}} \hat{G}_{\mathbf{k}} [Js + J^2(\Sigma^2 \hat{G}_j + \hat{X}_j)] \hat{G}_{\mathbf{k}'',\mathbf{k}'} \alpha_{j,\mathbf{k}''}$$

where $\hat{G}_j = N^{-1} \sum_{\mathbf{k}} \alpha_{j,\mathbf{k}}^2 \hat{G}_{\mathbf{k}}$, $\hat{X}_j = N^{-1} \sum_{\mathbf{k}} \alpha_{j,\mathbf{k}}^2 \hat{G}_{\mathbf{k}} (\varepsilon + h) \hat{X}_{\mathbf{k}}$, and its standard iteration yields in the result:

$$\hat{G}_{\mathbf{k},\mathbf{k}'} = N^{-1} \sum_j \alpha_{j,\mathbf{k}} \hat{G}_{\mathbf{k}} \hat{T}_j \hat{G}_{\mathbf{k}'} \alpha_{j,\mathbf{k}'}, \quad (4)$$

with the partial T-matrices $\hat{T}_j = [Js + J^2(\Sigma^2 \hat{G}_j + \hat{X}_j)][1 - Js - J^2(\Sigma^2 \hat{G}_j + \hat{X}_j)]^{-1}$. By the definition of our model,

the parameter Js is positive. It is interesting to trace the behavior of \hat{T}_j in the two characteristic limits for AFM correlations between Cu^{2+} spins.

In the paramagnetic limit: $h \rightarrow 0$, $s \rightarrow 0$, we have $\Sigma^2 \rightarrow S(S+1)/3$ and $\hat{X}_j \rightarrow 2S(S+1)/3 - N^{-1} \sum_{\mathbf{k}} \alpha_{j,\mathbf{k}}^2 (1 + 2\xi_{\mathbf{k}}/E_{\mathbf{k}}) \hat{G}_{\mathbf{k}} \hat{\tau}_3$. In neglect of the small last term we arrive at:

$$\hat{T}_j \rightarrow J^2 S(S+1) \hat{G}_j [1 - J^2 S(S+1) \hat{G}_j]^{-1}$$

generalizing the known results [6, 9] for the case of extended impurity center.

Another limit, fully polarized, $h \rightarrow \infty$, $s \rightarrow S$, corresponds to $\Sigma^2 \rightarrow 0$, $\hat{X}_j \rightarrow 0$ and results in

$$\hat{T}_j \rightarrow JS(1 - JS\hat{G}_j)^{-1} \quad (5)$$

which is only due to the effect of MF magnetic scattering. The obvious validity condition for this limit, $JS \gg k_{\text{B}}T$, well applies in the SC phase at $T < T_c \sim \Delta/k_{\text{B}}$, so we use Eq. 5 for the T-matrices in what follows.

The local SC correlation is characterized by the average $\Delta_{12} = 2V \langle a_{\delta_1, \downarrow} a_{\delta_2, \uparrow} \rangle$ (see Fig. 1) where a site operator $a_{\mathbf{n}, \sigma}$ is expressed through band operators: $a_{\mathbf{n}, \sigma} = N^{-1/2} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{n}} a_{\mathbf{k}, \sigma}$. Since the phase of $\Delta_{\mathbf{k}}$ is chosen zero, Δ_{12} is real. For $J = 0$, this average does not differ from the uniform gap parameter:

$$\Delta_{12} \rightarrow \frac{2V}{N} \sum_{\mathbf{k}} \langle a_{-\mathbf{k}, \downarrow} a_{\mathbf{k}, \uparrow} \rangle e^{i\mathbf{k} \cdot (\delta_2 - \delta_1)} = \Delta,$$

whereas for $J \neq 0$ the maximum perturbation of SC order near the impurity is given by the suppression parameter $\eta_{\text{sup}} = 1 - \Delta_{12}/\Delta$. Its value is confined between 0 (for pure SC) and 1 (for complete local suppression of SC order), and it only results from non-diagonal GF's:

$$\begin{aligned} \eta_{\text{sup}} &= \frac{2V}{N\Delta} \sum_{\mathbf{k}, \mathbf{k}' \neq \mathbf{k}} \langle a_{-\mathbf{k}, \downarrow} a_{\mathbf{k}', \uparrow} \rangle e^{i(\mathbf{k} \cdot \delta_2 - \mathbf{k}' \cdot \delta_1)} = \\ &= \frac{V}{2\pi\Delta} \sum_j (-1)^j \int_{-\infty}^0 d\varepsilon \text{Im Tr } \hat{G}_j \hat{T}_j \hat{G}_j \hat{\tau}_1, \end{aligned} \quad (6)$$

where the trace is in Nambu indices and Eqs. 3,4 were used. Expansion of \hat{G}_j in Pauli matrices only contains $\hat{\tau}_1$ terms at $j = 2, 3$ (by the parity of $\alpha_{j,\mathbf{k}}$ with respect to the permutation $k_x \leftrightarrow k_y$): $JS\hat{G}_{2,3} = A + B\hat{\tau}_3 \pm C\hat{\tau}_1$. Hence only $j = 2, 3$ actually contribute in Eq. 6 by

$$\eta_{\text{sup}} = \frac{V\varepsilon_{\text{F}}\rho_0^2}{4} \int_0^{\varepsilon_{\text{F}}} \frac{F(\varepsilon)}{\varepsilon} d\varepsilon, \quad (7)$$

where

$$F(\varepsilon) = \frac{16\varepsilon}{\pi JS\varepsilon_{\text{F}}\Delta\rho_0^2} \text{Im} \left[1 - \frac{1}{(1-A)^2 - B^2 - C^2} \right] C,$$

and the complex coefficients A, B, C as functions of energy are estimated in the relevant range $\Delta < \varepsilon < \varepsilon_{\text{F}}$,

setting $E_{\mathbf{k}} \approx \xi_{\mathbf{k}} \approx Wa(k^2 - k_{\text{F}}^2)/8$:

$$\begin{aligned} A &\approx \frac{JS\rho_0\varepsilon}{8} (\ln |\frac{\varepsilon_{\text{F}} + \varepsilon}{\varepsilon_{\text{F}} - \varepsilon}| + 2i\pi), \\ B &\approx \frac{JS\rho_0}{8} \ln \frac{\varepsilon_{\text{F}}^2 - \varepsilon^2}{(W - \varepsilon_{\text{F}})^2}, \\ C &\approx \frac{\pi JS\rho_0\varepsilon_{\text{F}}\Delta}{E\varepsilon} [\ln |\frac{\varepsilon_{\text{D}} + \varepsilon}{\varepsilon_{\text{D}} - \varepsilon}| + i\pi\theta(\varepsilon_{\text{D}} - \varepsilon)]. \end{aligned}$$

Numeric analysis of these expressions with realistic parameter values: $W \sim 2$ eV, $JS\rho_0 \sim 1$, $\varepsilon_{\text{F}} \sim 0.3$ eV, $\varepsilon_{\text{D}} \sim 0.15$ eV, shows that the main contribution into the integral, Eq. 7, comes from the BCS shell $\Delta < \varepsilon < \varepsilon_{\text{D}}$, where we have: $F(\varepsilon) \approx 1$, $0 < 1 - F(\varepsilon) \ll 1$, while $0 < -F(\varepsilon) \ll 1$ out of this shell, $\varepsilon_{\text{D}} < \varepsilon < \varepsilon_{\text{F}}$ (Fig. 2). Taking in mind the relation $\ln(\varepsilon_{\text{D}}/\Delta) \approx W/(V\gamma_m) = W^2/(4V\varepsilon_{\text{F}})$ which follows from Eq. 1, we obtain from Eq. 7 *almost complete* suppression: $\eta_{\text{sup}} \approx 1$. A small residual part $0 < 1 - \eta_{\text{sup}} \ll 1$ is only due to a small negative deviation of $F(\varepsilon)$ from unity within the shell and to a small negative out-of-shell contribution. Thus, for the above indicated choice of parameters we have $\eta_{\text{sup}} \approx 96\%$. The value of $1 - \eta_{\text{sup}}$ yet diminishes with growing JS , but it should be stressed that no unitary limit $JS\rho_0 \gg 1$ is needed to get such a strong effect.

The decay of this maximum effect with separation \mathbf{R} from the impurity is given, in similarity with Eq. 6, by

$$\eta_{\text{sup}}(\mathbf{R}) = \frac{V}{\pi\Delta} \int_{-\infty}^0 d\varepsilon \text{Im Tr } \hat{G}_2(\mathbf{R}) \hat{T}_2 \hat{G}_2(\mathbf{R}) \hat{\tau}_1, \quad (8)$$

Here the matrix $\hat{G}_j(\mathbf{R}) = N^{-1} \sum_{\mathbf{k}} e^{i\mathbf{k} \cdot \mathbf{R}} \alpha_{j,\mathbf{k}} \hat{G}_{\mathbf{k}}$, and for $R \gg \xi_{\pm} = a\sqrt{W/[8(\varepsilon_{\text{F}} \pm \varepsilon)]}$ it is mainly contributed by two saddle points in the complex k -plane: $\pm\xi_{\pm}^{-1} - iR^{-1}$, hence all its matrix elements decay asymptotically like $\cos(R/\xi_{\pm})/\sqrt{R/\xi_{\pm}}$, and the non-diagonal elements contain yet the anisotropic factor $(\Delta/\varepsilon) \cos 2\psi$ where $\psi = \arctan R_y/R_x$. However, for the energies $\varepsilon \sim \varepsilon_{\text{D}}$ relevant here, such anisotropy is less pronounced than that in the limit $\varepsilon \rightarrow 0$ considered by Balatsky *et al* [27]. Integration in Eq. 8 results in asymptotic $\eta_{\text{sup}}(\mathbf{R}) \approx \eta_{\text{sup}} \sqrt{W/(8\varepsilon_{\text{F}})} \sum_{i=\pm} (u_i + f_i \cos 2\psi + h_i \cos 4\psi)(a/R)$ where $h_i \ll f_i \sim u_i \sim 1$. This angular dependence resembles that for LDOS around Zn impurity, suggested by Haas and Maki from continuous Bogolyubov-de Gennes equations [28], while the anomalously slow radial decay should enhance the overall suppression of SC order.

Besides the considered local suppression of the order parameter, related to the non-diagonal (in Nambu indices) elements of GF's $\hat{G}_{\mathbf{k},\mathbf{k}'}$, there are also local effects related to their diagonal elements. Thus, the variation of local DOS (LDOS): $\rho(\mathbf{n}) = (\pi N)^{-1} \sum_{\mathbf{k}, \mathbf{k}' \neq \mathbf{k}} \text{Im Tr } e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{n}} \hat{G}_{\mathbf{k},\mathbf{k}'} \hat{\tau}_3$, attains its maximum at $\mathbf{n} = \delta$, nearest neighbor sites to the impurity, and Eq. 4 mainly contributes there by $j = 1$: $\rho(\delta) \approx \text{Im Tr } \hat{G}_1(\delta) \hat{T}_1 \hat{G}_1(\delta) \hat{\tau}_3$. The relevant GF's are

$\hat{G}_1(\delta) \approx 2N^{-1} \sum_{\mathbf{k}} \hat{G}_{\mathbf{k}} = 2(g_0 + g_3 \hat{\tau}_3)$, where $g_0 \approx \rho_0 \varepsilon [\varepsilon_F^{-1} + i(\pi/\Delta) \arcsin(\Delta/\varepsilon)]$ and $g_3 \approx \rho_0 \ln(W/\varepsilon_F)$ [3]. Considered as a function of energy, $\rho(\delta)$ displays a very sharp resonance in the denominator of \hat{T}_1 : $\text{Re}[1 - 2JSg_0(\varepsilon)]^2 - (2JSg_3)^2 \rightarrow 0$ at $\varepsilon \rightarrow 0$ (cf. Fig. 3) with the observed peak in the related tunnel conductivity [29] if the impurity perturbation parameter J is close to $J_{cr} = 1/(2Sg_3)$. This refers to a *fine tuned* rather than unitary perturbation J and agrees with its choice made to estimate η_{sup} . The $j = 1$ contribution also dominates in the Kondo-like local polarization of itinerant spins: $m(\delta) \approx \int_0^{\varepsilon_F} d\varepsilon \text{Im Tr } e^{i(\mathbf{k}-\mathbf{k}') \cdot \mathbf{n}} \hat{G}_1(\delta) \hat{T}_1 \hat{G}_1(\delta)$, which should explain the observed enhancement of exchange fields on ^{63}Cu [21] and ^{89}Y [17] nuclei close to Zn impurities. A more detailed treatment of these phenomena will be presented elsewhere.

The proposed model can be equally applied to isovalent substitutes for Cu, which are magnetic themselves, as Ni^{2+} or Fe^{2+} . But, since the net MF on neighbor O sites in this case is due to incomplete AFM compensation of exchange fields by different magnetic ions, the perturbation parameter JS may be *weaker* than that for non-magnetic Zn^{2+} and so the resulting suppression of

SC order, as is observed in the experiment [11].

In conclusion, we developed a microscopic model of spin dependent perturbation on charge carriers in CuO_2 planes, produced by a non-magnetic substitute for Cu. An almost complete suppression of *d*-wave order parameter at nearest neighbor sites to the impurity atom is obtained, as a result of parallel alignment of carrier spins in the exchange field JS by non-compensated Cu^{2+} spins, and this strong effect is achieved with moderate JS values. It decays with distance from impurity rather slowly, which can explain the fast destroying of SC order in cuprates already at low Zn concentration. The model also provides explanation for other local effects, such as a sharp resonance of LDOS and local polarization of charge carrier spins close to impurity.

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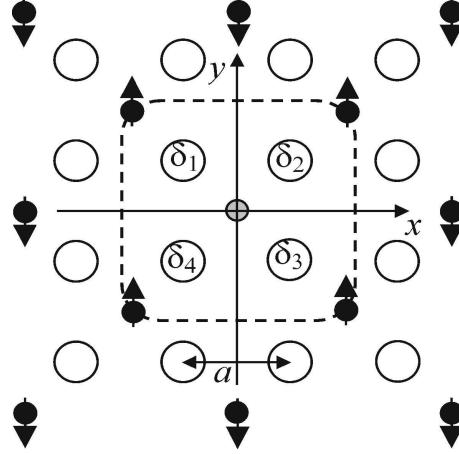


Figure 1: Effective magnetic perturbation for charge carriers on nearest neighbor sites δ_i to the non-magnetic impurity substitute (grey circle) for Cu^{2+} in CuO_2 plane

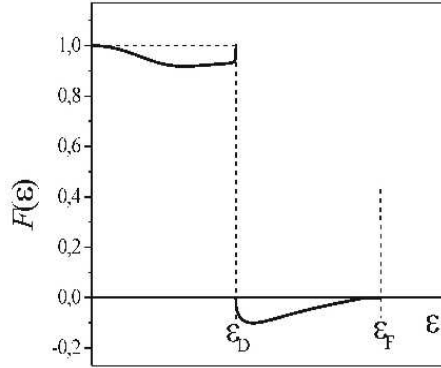


Figure 2: The function $F(\varepsilon)$ for parameter values $W = 2$ eV, $JS\rho_0 = 1$, $\varepsilon_F = 0.3$ eV, $\varepsilon_D = 0.15$ eV (the discontinuity is due to the assumed sharp BCS-shell boundary).

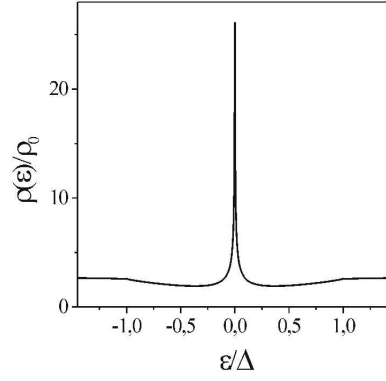


Figure 3: Local DOS on nearest neighbor O sites to Zn impurity site, as a function of energy $\rho(\varepsilon)$, presents a sharp zero-energy resonance at the choice of perturbation parameter $JS\rho_0 = 1.26 \approx J_{cr}S$.